Materials Computation Center, University of Illinois

Duane Johnson and Richard Martin, NSF DMR-9976550

Machine-learning to Perform Multi-timescale Kinetic Modeling

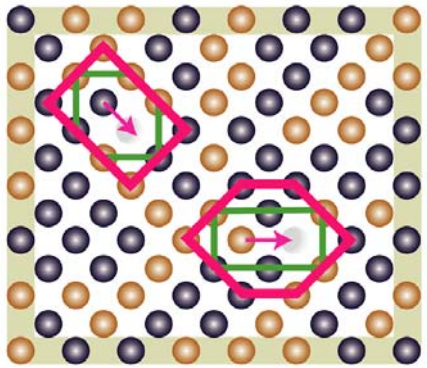
from co-PIs: Duane Johnson and David Goldberg

Research

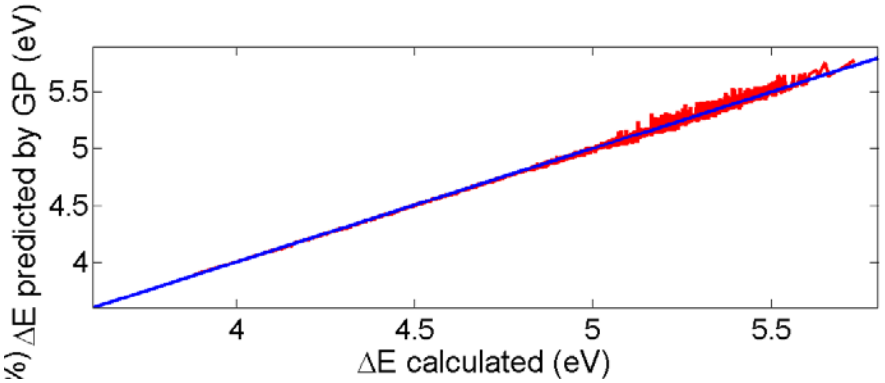
Experiments can measure kinetic processes from milliseconds to seconds in materials, whereas Molecular Dynamics simulates kinetics up to nanoseconds, even using parallel supercomputers! How can atomic processes (barriers) that control kinetics be calculated and followed to real times?

We devised a machine-learning strategy to get barriers based on concepts of evolution - Genetic Algorithms (GA). Genetic Programming (GA that evolve computer programs) is used to learn functions that fit a limited set of calculated barriers and then predicts all others. For example, atomic diffusion at the surface of a binary alloy is determined by barriers affected by surface structure, number of vacancies and differing atom arrangements — which are so enormous in number that no direct calculation is possible in real materials. We machine-learn the barriers (saving large CPU time) and use Kinetic Monte Carlo methods to simulate real experimental times.

Submitted to *Physical Review Letters* by graduate student K. Sastry, April 2003.



Kinetic modeling: A surface of a binary alloy with two vacancies (missing atoms) showing a first and second nearest neighbor (n.n.) diffusion paths with first (green box) and second (red box) n.n. chemical arrangements.



Predictions vs. calculations: The GP-predicted (red) versus calculated energy barriers (blue) for 8196 barriers at surface of fcc $Cu_{50}Co_{50}$ alloy. GP used as few as 25 barriers to learn all barriers, through the creation of a complex fitting function. Simple basis-set regression is not possible .